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Nitro-functionalized Bis(pyrazolate) Metal–Organic Frameworks as Carbon Dioxide Capture Materials under Ambient Conditions

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Abstract

© 2018 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim The metal–organic frameworks (MOFs) M(BPZNO2) (M=Co, Cu, Zn; H2BPZNO2=3-nitro-4,4′-bipyrazole) were prepared through solvothermal routes and were fully investigated in the solid state. They showed good thermal stability both under a N2 atmosphere and in air, with decomposition temperatures peaking up to 663 K for Zn(BPZNO2). Their crystal structure is characterized by 3D networks with square (M=Co, Zn) or rhombic (M=Cu) channels decorated by polar NO2 groups. As revealed by N2 adsorption at 77 K, they are micro-mesoporous materials with BET specific surface areas ranging from 400 to 900 m2 g−1. Remarkably, under the mild conditions of 298 K and 1.2 bar, Zn(BPZNO2) adsorbs 21.8 wt % CO2 (4.95 mmol g−1). It shows a Henry CO2/N2 selectivity of 15 and an ideal adsorbed solution theory (IAST) selectivity of 12 at p=1 bar. As a CO2 adsorbent, this compound is the best-performing MOF to date among those bearing a nitro group as a unique chemical tag. High-resolution powder X-ray diffraction at 298 K and different CO2 loadings revealed, for the first time in a NO2-functionalized MOF, the insurgence of primary host–guest interactions involving the C(3)–NO2 moiety of the framework and the oxygen atoms of carbon dioxide, as confirmed by Grand Canonical Monte Carlo simulations. This interaction mode is markedly different from that observed in NH2-functionalized MOFs, for which the carbon atom of CO2 is involved.

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Keywords

adsorption, host–guest interactions, metal–organic frameworks, N ligands, X-ray diffraction

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